Metallic Precipitate Contribution to Generation and Recombination Currents in p-n Junction Devices via the Schottky Effect

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ABSTRACT

The contribution of metal and metal-silicide precipitates to recombination and to generation currents has been modeled for silicon based pn junctions. The physical mechanism responsible for the electrical activity of the metallic precipitate is assumed to arise from the Schottky junction property between the precipitate and the Si matrix material, with the precipitate located in the charge depletion region of the structure. It is found that the precipitate changes from a highly effective carrier recombination center to a carrier generation center when the junction bias is changed from forward to reverse biasing conditions in steady states. Based on the physical model, numerical simulation results showed that the precipitates behave electrically like Shockley-Hall-Read recombination or generation centers but with an enhanced activity. The dependence of the device current on the Schottky barrier height between the hosting semiconductor and the silicide forming the precipitate and doping levels have also been investigated.

1. Introduction

To model the electrical activity of metallic precipitates inside the depletion region of the p-n junction, a cylindrical diode, 2μ in length and 2μ in diameter, with the p-n junction at the middle of its long dimension, is considered (Fig 1a). A spherical precipitate 100Å in diameter is placed at the n-side of the depletion region of the diode along its center of rotation. The cylindrical symmetry of the diode and the spherical symmetry of the precipitate allowed the problem to be formulated and solved for a longitudinal planar section passing through the center of the precipitate, see Fig.1b. This enables a steady-state two-dimensional model of the p-n junction to be used instead. To account for the metal-Si junction property, the Schottky effect model [1] is used.

2. Formulation of Problem

Physically, we note that the precipitate charges-up with the same charge as the majority carrier and creates its own electric field. This field on the one hand, and the p-n junction field together with the gradients of carrier concentrations on the other, balance each other so that a steady state is reached. Which factor is dominant is strongly dependent on the bias condition and will be made clear in the solution of the problem. The precipitate charge influences little the depletion region charge distribution because the amount of charges accumulated on the precipitate surface is small. However, the overall effect of the charged precipitate on the device band structure and carrier transport phenomena in the depletion region can be very strong because this charge is confined in the very small volume of the precipitate, and hence the electric field emerging or entering the precipitate has values comparable with the electric field of the p-n junction itself.

A set of the standard steady-state semiconductor equations with dependent variables (ϕ_e,ϕ_h,ψ), where ϕ_e, ϕ_h are the electron and hole quasi-Fermi levels respectively and ψ is the electric potential, have been used as governing equations for the carrier transport phenomena in Si, while the boundary conditions at the Si-metal interface have been derived from the thermionic emission theory described in detail elsewhere [2]. The mathematical model consists of two continuity equations and Poisson's equation posed in the bounded domain representing the device geometry with two ohmic contacts and the Si-metal interface [3].

3. Results and Discussion

The problem has been solved numerically using a general-purpose two-dimensional finite-element solver. The materials parameters used in the simulation are summarized in Table 1. The carrier profiles, the structure of quasi-Fermi levels, and electric potentials demonstrated that the precipitate charges with the same charge as the majority carrier in Si. In steady state, the precipitate, in our case charged negatively, creates its own electric field, which repels majority carriers and attracts minority carriers.

In transition from reverse bias to forward bias the effect of precipitate dynamically changes. As the device goes from reverse to forward bias the precipitate discharges and consequently the precipitate charge generated electric field decreases. Reverse biasing leads to the injection of carriers from metal into Si. Thus, under forward and reverse biasing conditions, the precipitate serves respectively as carrier recombination and generation centers.

The perturbation in the electric potential induced by the distribution of charge around the precipitate is small in the sense that it is confined inside space-charge region. Figure 2 shows a planar distribution of potential in the device space-charge region and Fig. 3 the potential along a line parallel to device current flow passing through the center of the precipitate. One can note that the potential outside the charge depletion region for the device without and with precipitate coincide. Although the potential variation induced by the charge on the precipitate surface is small, the electric field around the precipitate is very intense, almost spike-like (not shown) and hence tremendously enhancing its electric activity. This is because the potential variation due to the precipitate is confined in a small region surrounding the spherical precipitate with a radius less than 20 nm.

The total current density at the device contacts is shown respectively in Fig. 4 and Fig. 5 for forward bias up to 0.65V and for reverse bias up to -0.25V. The precipitate concentration has been varied by adjusting the diode volume (radius Ly), while the diode length 2Lx was kept constant to avoid altering the physics of the device space charge region. The current density has been plotted for the device without the precipitate but containing classical Shockley-Hall-Read (SRH) recombination or generation centers in a concentration giving a lifetime of about 10^{-8} sec on both sides (continuous line), and for two circular diodes having the same SRH recombination/generation center densities with different radii (dotted line) corresponding to a precipitate concentration of about $3.18\times10^{11}cm^{-3}$ for Ly = Lx and respectively for a precipitate concentration of about $1.9\times10^{10}cm^{-3}$ for Ly = 4Lx. As the metallic precipitates concentration decreases from the higher limit of the studied range (Ly = Lx) to the lower limit (Ly = 4Lx), the recombination or generation current drawn or generated by the precipitate decreases (see Fig. 4 and Fig. 5). The analyzed range is limited at the lower concentration by the efficiency of the numerical problem (the extension of the spatial domain of the problem in the direction perpendicular on the direction of the current flow becomes too large and consequently the computing time and resources increase drastically), and also has a higher limit because for very small radius of the circular device, the boundary conditions imposed on the exterior of the cylinder (reflection conditions), especially the electric field reflected on the exterior walls interact with the electric field created by the charge distribution due to the metallic precipitate. The presented I-V characteristics indicate that the precipitates behave electrically like enhanced activity SRH centers. In other words, they draw or generate a current proportional to $\exp\left(-\frac{V_a}{nk_BT}\right)$ where n is the ideality factor close to 2 and slightly dependent on the Schottky barrier height between the semiconductor and the metal or metal silicide forming the precipitate.

The current density as a function of Schottky barrier between silicon and metallic precipitate has been next investigated (see Fig. 6). The dotted line represents the value of the current density when there is no precipitate. For a Schottky barrier less than 0.3 eV, the current through the device without and with precipitate has the same value, as expected. The most intense electric activity of the precipitate should be seen for a Schottky barrier height equal to about half of the silicon bandgap, 0.56 eV, when both charge carriers can enter or emerge from the precipitate surface equally probable. The simulation results in Fig. 6 show that indeed precipitate electric activity has a maximum around 0.56 eV. All transition metal silicides except Ti have Schottky barrier heights close to 0.56 eV [4], so their electric activity is high.

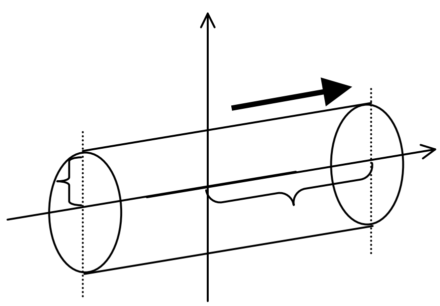
The variation of the current density as a function of Schottky barrier height between silicon and metallic precipitate, with n doping concentration as a parameter is also presented in Fig. 6, with N_d^+ between $5\times10^{15}cm^{-3}$ and $1\times10^{17}cm^{-3}$. The effect of Schottky barrier height variation on the current through the p-n junction is more pronounced for low doping concentrations and decreases as the doping level increases. For high doping levels of the n-type substrate, the difference between precipitates having different Schottky barriers tends to flatten down (see Fig. 6). Also, the efficiency of the precipitate as a recombination center drastically decreases when doping level increases. When N_d^+ changes from $5\times10^{15}cm^{-3}$ to $1\times10^{17}cm^{-3}$, the ratio of the maximum current through the device with the precipitate to the current through the device without the precipitate changes from 141 to about 5.

Finally the multiple-precipitate case is considered. Two identical precipitates were symmetrically placed on the n-side and p-side 75 nm away from the junction along the rotation axis of the device with a device radius of 1 μm. The material related parameters used in this simulation are listed in Table 2 and the carrier profiles for a forward bias of 0.2 V is shown in Fig. 7. The results show that for the same doping levels, $N_d^+ = N_a^- = 5\times10^5$ cm^{-3}, the current through the device having a precipitate within the n-side space-charge region is almost equal to the current through the device with the same precipitate within the p-side space-charge region. The forward current-voltage characteristic has been plotted for the device containing one and two precipitates (see Fig. 8). This shows that the total current density through the device is almost the same when the precipitate is moved from n-side space-charge region to p-side space-charge region, and is about twice when it contains two similar precipitates on both sides. The device current is proportional to the precipitate concentration.

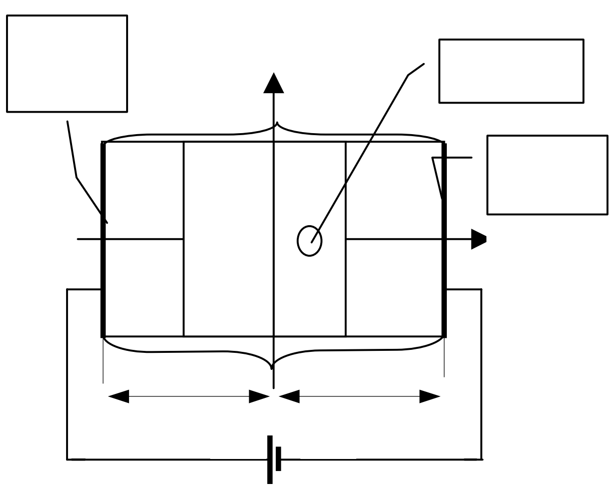
In conclusion, the electric activity of the metallic precipitate is dictated by the operating regime of the p-n junction. The precipitate dynamically turns from a generation center in a reverse biased p-n junction to a recombination center in a forward biased junction. Consequently, the presence of the precipitate in the depleted region of a reverse biased pn junction increases the leakage current and also increases the forward current for a forward biased pn junction. The metallic precipitate has an electric activity similar to a SRH center (n = 2 current proportional to precipitate density).

Table 1. Material parameters

Parameter	Value
p-side doping, N_a^-	$4.5\text{x}10^{15}$ cm^{-3}
n-side doping, N_d^+	$1\text{x}10^{16}$cm^{-3}
Hole lifetime, τ_p	$1\text{x}10^{-8}$ sec
Electron lifetime, τ_n	$1\text{x}10^{-8}$ sec
Precipitate radius, R_p	$5\text{x}10^{-7}$ cm
Schottky barrier height between Si and silicide ϕ_{Bn}	0.68 V



a)



b)

Figure 1. Schematic diagram of the device. a) 3D view of the device used in simulation. b) longitudinal section through the center of precipitate.

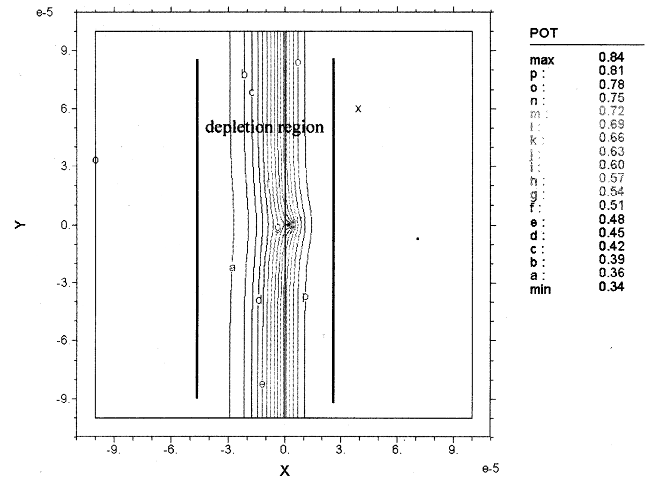


Figure 2. Planar potential distribution in p-n junction space charge region for a forward bias of 0.2 V.

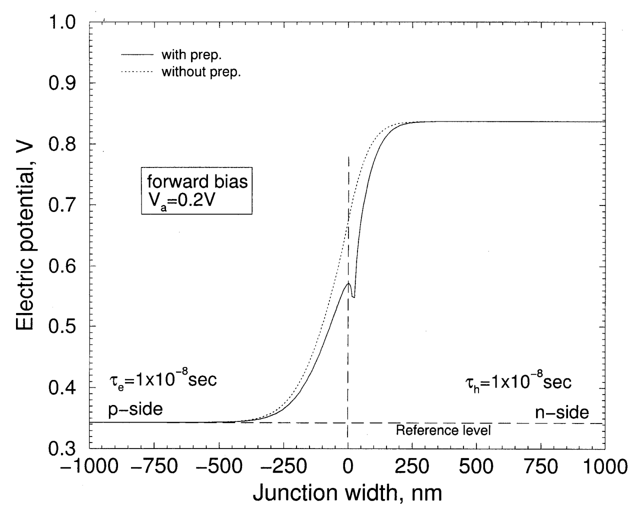


Figure 3. Potential distribution in p-n junction space charge region for a forward bias of 0.2 V along a line parallel to current flow and passing though the center of the precipitate.

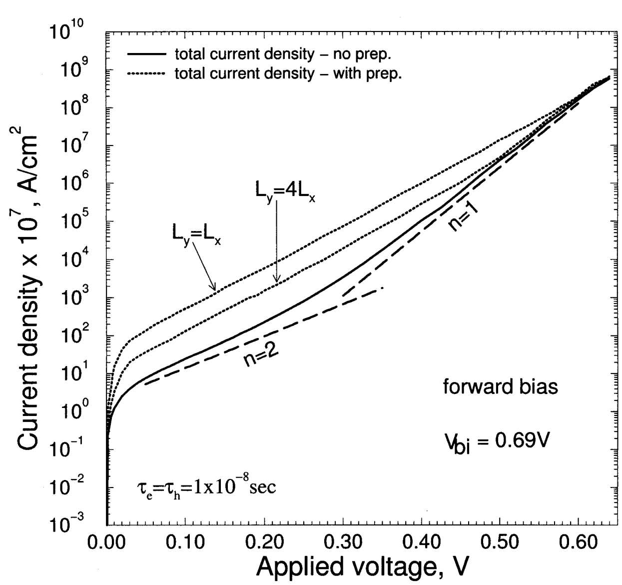


Figure 4. P-n junction current density under forward bias.

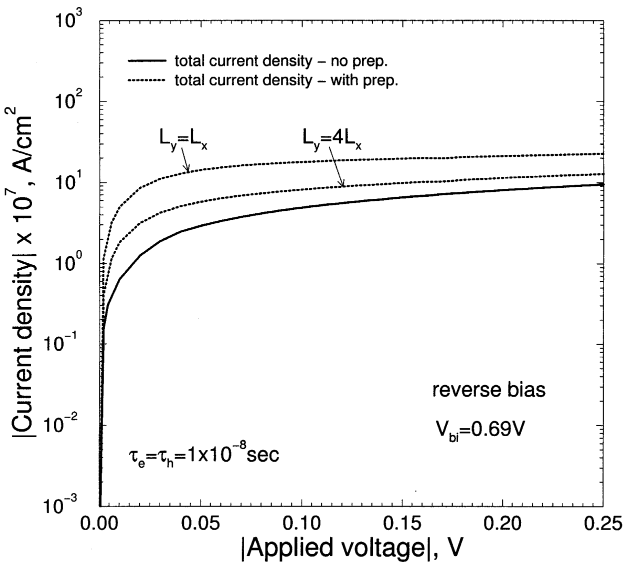


Figure 5. P-n junction current density under reverse bias.

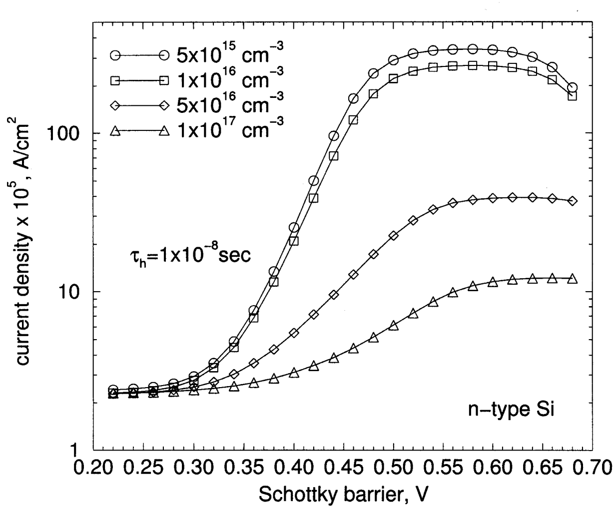


Figure 6. Dependence of current density on Schottky barrier and doping level.

Table 2. Material parameters

Parameter	Value
p-side doping, N_a^-	5×10^{15} cm^{-3}
n-side doping, N_d^+	5×10^{15} cm^{-3}
Hole lifetime, τ_p	1×10^{-7} sec
Electron lifetime, τ_n	1×10^{-7} sec
Precipitate radius, R_P	5×10^{-7} cm
Schottky barrier height between Si and metal ϕ_{Bn}	0.68 V

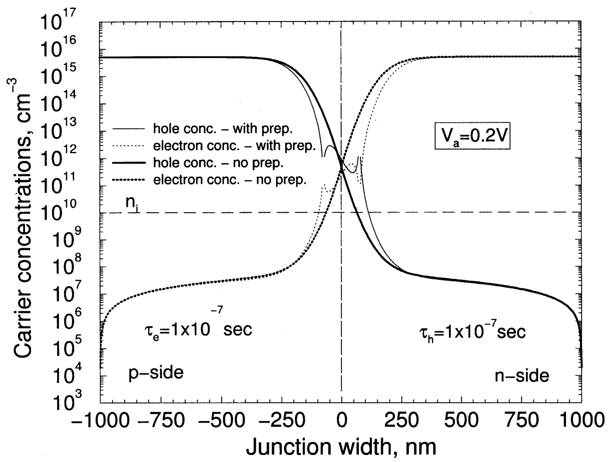


Figure 7. Carrier profiles for the p-n junction with two precipitates symmetrically placed on the two sides of the device, 70 nm away from the junction.

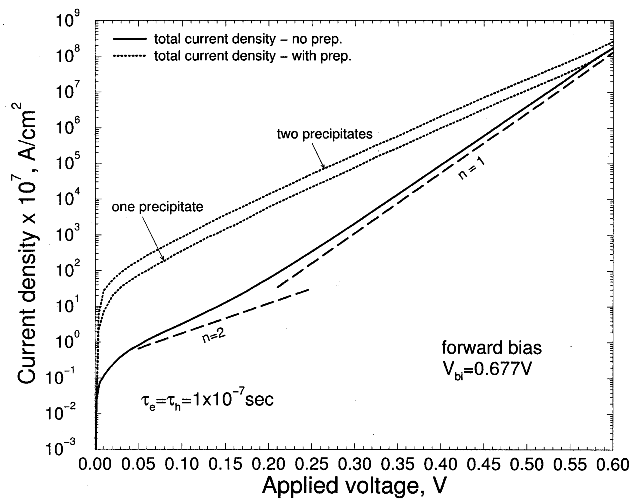


Figure 8. P-n junction current density under forward bias – multiple-precipitate case.

References

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